Large deviations of heat flow in harmonic chains

Anupam Kundu, Sanjib Sabhapandit, and Abhishek Dhar

Raman Research Institute, Bangalore 560080, India

Abstract. We consider heat transport across a harmonic chain connected at its two ends to white-noise Langevin reservoirs at different temperatures. In the steady state of this system the heat Q flowing from one reservoir into the system in a finite time τ has a distribution $P(Q, \tau)$. We study the large time form of the corresponding moment generating function $\langle e^{-\lambda Q} \rangle \sim g(\lambda) \, e^{\tau \mu(\lambda)}$. Exact formal expressions, in terms of phonon Green's functions , are obtained for both $\mu(\lambda)$ and also the lowest order correction $g(\lambda)$. We point out that, in general a knowledge of both $\mu(\lambda)$ and $g(\lambda)$ is required for finding the large deviation function associated with $P(Q, \tau)$. The function $\mu(\lambda)$ is known to be the largest eigenvector of an appropriate Fokker-Planck type operator and our method also gives the corresponding eigenvector exactly.

1. Introduction

Among the most interesting recent developments in the theory of nonequilibrium processes are the so-called fluctuation theorems [1, 2, 3, 4, 5, 6, 7]. These theorems make quantitative statements on the probability of negative entropy production in nonequilibrium systems. They have been theoretically [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19] and experimentally [20, 21, 22, 23, 24, 25, 26, 27, 28] studied in a large number of systems in various nonequilibrium states. The results have been obtained both in the context of transient and steady state phenomena. In the case of nonequilibrium steady states in systems carrying heat or particle current, the fluctuation theorems have pointed to the importance of the large deviation function (LDF) and the cumulant generating function (CGF) [29]. The steady state fluctuation theorem can, in these cases, be equivalently stated as a symmetry property of the LDF or the CGF [12, 14, 15]. Apart from their interest from the point of the fluctuation theorem these two functions contain important information on nonequilibrium processes: the LDF gives the precise probability of the occurrence of rare events while the CGF contains information on the average current in a system as well as all moments [29]. So far there are very few examples where either the LDF or the CGF have been exactly computed. The few examples include particle transport in exclusion processes [12, 14, 15], Brownian motors [18, 19], power dissipation and heat transport in single Brownian particles [16, 30, 31, 32] and heat conduction across a quantum harmonic chain [17].

Consider the example of heat conduction through a system coupled to two heat baths at different temperatures T_L and T_R and let Q be the heat flowing from the left reservoir into the system during a time interval τ. Then Q is a stochastic variable with a distribution $P(Q)$ and the LDF and CGF for this problem are defined by the following scaling forms, valid for large τ:

$$P(Q, \tau) \sim e^{-\tau h(Q/\tau)}$$
$$Z(\lambda) = \langle e^{-\lambda Q} \rangle = \int_{-\infty}^{\infty} dQ \, e^{-\lambda Q} \, P(Q, \tau) \sim g(\lambda) \, e^{\tau \mu(\lambda)}. \quad (1)$$

We will refer to $h(q)$ and $\mu(\lambda)$ as the LDF and CGF respectively. For large τ the term $g(\lambda)$ is a correction to the CGF and can normally be ignored in the saddle-point calculation which relates $h(q)$ and $\mu(\lambda)$. The saddle-point calculation gives:

$$h(q) = -[\mu(\lambda^*) + q\lambda^*], \qquad \mu'(\lambda^*) = -q \ . \quad (2)$$

While the LDF and the CGF are normally related by Legendre transformations, there are several examples where this relation is known to break down. This happens if the function $g(\lambda)$ has singularities in the region of the saddle-point integration. Interestingly, in such cases, the CGF might still satisfy the fluctuation symmetry relation, while the LDF does not [16, 32, 33]. Thus we note that if one is interested in the LDF then it is in general important to calculate both $\mu(\lambda)$ and the leading correction term $g(\lambda)$. Of course $\mu(\lambda)$ is itself of interest since it contains important information on current and current-noise properties and relations between response functions.

The aim of this paper is to present a formalism to obtain $\mu(\lambda)$ as well as $g(\lambda)$ for the problem of heat conduction across a harmonic chain connected to white-noise Langevin heat baths. We use the linearity of the problem and show that the problem of finding the generating function $Z(\lambda)$ reduces to performing multi-dimensional Gaussian integrations. We are able to find a closed form expression for $\mu(\lambda)$, as given by (11), in terms of the phonon-transmission function, a well known quantity in the study of heat conduction in harmonic systems. Finding $g(\lambda)$ is more difficult but we are able to also express it, as given by (59), in terms of appropriate phonon Green's functions. For the case of a single free Brownian particle we can use our approach to explicitly obtain both $\mu(\lambda)$ and $g(\lambda)$ and for this case we recover the results of Visco [16], obtained by solving the Fokker-Planck equation.

The paper is organized as follows. In Sec. (2) we define the model that we study, make some general remarks on the problem of computing the generating function for heat, and briefly explain our method. In Sec. (3) we give the calculation of the CGF $\mu(\lambda)$ while in Sec. (4) we give the calculation of the correction term $g(\lambda)$. The example of a single Brownian particle, for which explicit results for $\mu(\lambda)$ and $g(\lambda)$ can be obtained, are considered in Sec. (5). Finally we discuss our results in Sec. (6).

2. Model and general considerations

We consider a one-dimensional chain of N particles with harmonic interactions and described by the Hamiltonian:

$$\mathcal{H} = \sum_{l=1}^{N} \frac{1}{2} m_l v_l^2 + \frac{1}{2} \sum_{l=1}^{N} \sum_{m=1}^{N} \boldsymbol{\Phi}_{lm} x_l x_m, \tag{3}$$

where x_l, v_l and m_l are, respectively, the displacement about the equilibrium position, velocity and mass of lth particle and the matrix $\boldsymbol{\Phi}$ represents the force matrix of the system. For the moment we assume that at least one site of the chain is pinned so that the centre of mass attains a steady state distribution. However, later we show that the results are also valid for a free harmonic chain. The particles 1 and N at the two ends — which we refer as left (L) and right (R) respectively — are coupled to white noise Langevin heat reservoirs at two different temperatures T_L and T_R respectively. The system, described by the variables $X^T = (x_1, x_2, \ldots, x_N)$ and $V^T = (v_1, v_2, \ldots, v_N)$, evolves according to the following equations of motion:

$$\dot{X} = V, \quad \boldsymbol{M}\dot{V} = -\boldsymbol{\Phi}X - \boldsymbol{\gamma}V + \eta(t), \tag{4}$$

where $\boldsymbol{M} = \text{diag}(m_1, m_2, \ldots, m_N)$ is the mass matrix, the dissipation matrix $\boldsymbol{\gamma}$ has matrix elements $\boldsymbol{\gamma}_{i,j} = \delta_{i,j}(\delta_{i,1}\gamma_L + \delta_{i,N}\gamma_R)$ and the noise vector η has elements $\eta_i(t) = \delta_{i,1}\eta_L(t) + \delta_{i,N}\eta_R(t)$. The variables $\eta_L(t), \eta_R(t)$ are zero-mean Gaussian white noises with correlations given by:

$$\langle \eta_\alpha(t)\eta_{\alpha'}(t') \rangle = 2\delta_{\alpha,\alpha'} \, d_\alpha \, \delta(t-t') \,, \quad \text{where } d_\alpha = \gamma_\alpha T_\alpha \,, \quad \alpha, \alpha' = L, R \,. \tag{5}$$

and we have set the Boltzmann constant $k_B = 1$.

Since the equations of motion (4) are linear and the noise vector η is Gaussian, the probability distribution function of the phase space variables $U^T = (X^T, V^T)$ in the nonequilibrium steady state is a Gaussian with mean $\langle U \rangle = 0$ and with covariance matrix $\lim_{t\to\infty}\langle UU^T \rangle$. We denote the nonequilibrium steady state distribution by $P_{\mathrm{SS}}(U)$. The covariance matrix of the ordered harmonic chain was obtained exactly in [34]. For mass-disordered systems the covariance matrix can be expressed in terms of phonon Green's functions [35, 36] . The quantity of our interest here is the total amount of heat, Q, flowing from one of the reservoirs —say the left (L) — into the system in a given time duration τ, in the nonequilibrium steady state. This is given by

$$Q = \int_0^\tau [\eta_L(t) - \gamma_L v_1(t)]v_1(t)\; dt, \tag{6}$$

where $v_1(t)$ evolves according to (4), with the initial condition at $t = 0$ drawn from the nonequilibrium steady state distribution. Clearly, Q is a fluctuating quantity whose value depends on the initial conditions $U_0 = U(t = 0)$ and the noise trajectory $\{\eta(t) : 0 \le t \le \tau\}$ during any particular realization. Let $P(Q, \tau)$ denote the probability distribution of Q and let $Z(\lambda) = \langle e^{-\lambda Q}\rangle$ be the corresponding characteristic function, where $\langle...\rangle$ denotes an average over initial configurations as well as over different paths.

It is useful to consider the restricted characteristic function $Z(\lambda, U, \tau|U_0) = \langle e^{-\lambda Q}\rangle_{U_0, U}$ where the expectation is taken over all trajectories of the system that evolve from a given initial configuration U_0 to a given final configuration U in time τ. As shown in Appendix A, this satisfies a Fokker-Planck-type equation:

$$\partial_\tau Z(\lambda, U, \tau|U_0) = \mathcal{L}_\lambda Z(\lambda, U, \tau|U_0)\;, \tag{7}$$

with the initial condition $Z(\lambda, U, 0|U_0) = \delta(U - U_0)$. The solution of this can formally be written down in the eigenbases of the Fokker-Planck operator $\mathcal{L}_\lambda$, and the large τ behavior is dominated by the term having the largest eigenvalue $\mu(\lambda)$, i.e.,

$$Z(\lambda, U, \tau|U_0) \sim \chi(U_0, \lambda)\Psi(U, \lambda)\; \exp[\tau\mu(\lambda)] \tag{8}$$

where $\Psi(U, \lambda)$ is the eigenfunction corresponding to the largest eigenvalue, *i.e.*, $\mathcal{L}_\lambda\Psi(U, \lambda) = \mu(\lambda)\Psi(U, \lambda)$, and $\chi(U_0, \lambda)$ is the projection of the initial state onto the eigenstate corresponding to the eigenvalue $\mu(\lambda)$. We note that for $\lambda = 0$, $Z(\lambda = 0, U, \tau|U_0)$ is just the phase space distribution at time τ. Hence the existence of a unique nonequilibrium steady state, which has been proved for this system [36], requires that $Z(\lambda = 0, U, \tau \to \infty|U_0) = P_{\mathrm{SS}}(U)$ and this implies that $\mu(0) = 0$, $\chi(U_0, 0) = 1$ and $\Psi(U, 0) = P_{\mathrm{SS}}(U)$. Using (8), and the fact that $P_{\mathrm{SS}}(U) = \Psi(U, 0)$, we get for large τ:

$$Z(\lambda) = \int dU_0 \int dU\, \Psi(U_0, 0)Z(\lambda, U, \tau|U_0) \sim g(\lambda)\; \exp[\tau\mu(\lambda)], \tag{9}$$

$$\text{where } g(\lambda) = \int dU_0\; \Psi(U_0, 0)\; \chi(U_0, \lambda) \int dU\; \Psi(U, \lambda)\;.$$

Note that $g(0) = 1$. As discussed in the introduction the large deviation function $h(q = Q/\tau) = -\lim_{\tau\to\infty} \ln P(Q, \tau)/\tau$ is given by the the Legendre transformation,

$$h(q) = -\Big[\mu(\lambda^*) + \lambda^* q\Big], \tag{10}$$

with $\lambda^*(q)$ implicitly given by the saddle point equation $\mu'(\lambda^*) = -q$. The above relation holds *provided* that $g(\lambda)$ is analytic along the real λ in the region $[0, \lambda^*]$, so that $g(\lambda)$ can be neglected in the saddle-point calculation as a subleading contribution and the contour of integration can be deformed smoothly through the saddle point λ^*. On the other hand, if $g(\lambda)$ possesses any singularity in the region $[0, \lambda^*]$, then the contour of the integration cannot be deformed smoothly through the saddle point λ^*, and one needs to include the singular part of $g(\lambda)$ in the saddle point calculation.

The calculation of the LDF thus requires one to compute the CGF $\mu(\lambda)$ and the leading correction $g(\lambda)$. From the above discussion we see that these can be obtained from the largest eigenvalue and eigenvector of an appropriate Fokker-Planck operator for this system. This is however very difficult in most cases, including for the model studied here. However the linearity of the dynamics and the Gaussian nature of the noise in the present problem allow the computation of $\mu(\lambda)$ and $g(\lambda)$ using a different approach. The basic idea we use is that the variable of interest Q is a quadratic function of the initial phase-space configuration U_0 and the noise-trajectories $\{\eta(t) : 0 \leq t \leq \tau\}$, both of which are Gaussian distributed variables. Hence the problem of computing $\langle e^{-\lambda Q} \rangle$ reduces to one of doing a multi-variate Gaussian integration. In the following sections we present the details.

We make some remarks on the symmetry property of the CGF. In general, if the operator $\mathcal{L}_\lambda$ and its adjoint $\mathcal{L}_\lambda^\dagger$ possess the symmetry $\mathcal{L}_\lambda^\dagger = \mathcal{L}_{a-\lambda}$, then it immediately follows that $\mu(\lambda) = \mu(a - \lambda)$. Even if another operator $\mathcal{L}'_\lambda$ — which is related to $\mathcal{L}_\lambda$ by a similarity transformation — possesses the symmetry $\mathcal{L}'^\dagger_\lambda = \mathcal{L}'_{a-\lambda}$, then also $\mu(\lambda)$ has the above symmetry. There are some examples of systems with Markovian dynamics where the evolution operator satisfies this property but this does not seem to be the case for the model discussed here. In fact, even for the simplest case of a single free Brownian particle connected to two heat reservoirs [16], the Fokker-Planck operator does not possesses the above mentioned symmetry. In this case however, the Fokker-Planck operator can be transformed to a Hermitian operator of a quantum harmonic oscillator where the potential remains invariant under $\lambda \to (\Delta\beta - \lambda)$. We are not aware of such a transformation for a system having more than one particle and hence the symmetry of $\mu(\lambda)$ is a non-trivial one.

3. Calculation of CGF $\mu(\lambda)$

Before giving the details of the calculation we first state our main result of this section for the CGF which is:

$$\mu(\lambda) = -\frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega \, \ln\left[1 + \mathcal{T}(\omega) T_L T_R \, \lambda(\Delta\beta - \lambda)\right], \tag{11}$$

where $\Delta\beta = T_R^{-1} - T_L^{-1}$ and

$$\mathcal{T}(\omega) = 4\gamma_L \gamma_R \omega^2 \boldsymbol{G}_{1,N}^+(\omega) \boldsymbol{G}_{1,N}^-(\omega), \tag{12}$$

$$\text{with} \quad \boldsymbol{G}^\pm(\omega) = \left[\boldsymbol{\Phi} - \omega^2 \boldsymbol{M} \pm i\omega\boldsymbol{\gamma}\right]^{-1}, \tag{13}$$

Note that $\boldsymbol{G}^-(\omega) = \boldsymbol{G}^+(-\omega) = \boldsymbol{G}^{+*}(\omega)$ (* denotes complex conjugate). Using (11), one can immediately verify the expression for the average energy current,

$$\lim_{\tau \to \infty} \frac{\langle Q \rangle}{\tau} = -\mu'(0) = \frac{T_L - T_R}{4\pi} \int_{-\infty}^{\infty} d\omega \, \mathcal{T}(\omega). \tag{14}$$

which was obtained previously [37, 36, 38, 39]. From (11), we note that $\mu(0) = 0$ as required. It is also evident that (11) possesses the symmetry $\mu(\lambda) = \mu(\Delta\beta - \lambda)$. We also note that (11) agrees with the classical limit of the result obtained in [17] for a quantum chain.

We now give the details of the derivation of the expression (11). We solve the Langevin equations of motion by Fourier transforms. Let us define the finite-time Fourier transforms and their inverses as follows:

$$\{\widetilde{X}(\omega_n), \widetilde{V}(\omega_n), \widetilde{\eta}(\omega_n)\} = \frac{1}{\tau} \int_0^\tau dt \, \{X(t), V(t), \eta(t)\} \exp(-i\omega_n t)$$

$$\{X(t), V(t), \eta(t)\} = \sum_{n=-\infty}^{\infty} \{\widetilde{X}(\omega_n), \widetilde{V}(\omega_n), \widetilde{\eta}(\omega_n)\} \, \exp(i\omega_n t)$$

$$\text{with } \omega_n = \frac{2\pi n}{\tau} \, . \tag{15}$$

The Gaussian noise configurations represented by $\{\eta(t) : 0 < t < \tau\}$, can now equivalently be described in the frequency domain, by the infinite sequence $\{\widetilde{\eta}(\omega_n) : n = -\infty, \ldots, -1, 0, \ldots, \infty\}$ of Gaussian random variables having the correlations

$$\langle \widetilde{\eta}_\alpha(\omega) \widetilde{\eta}_{\alpha'}(\omega') \rangle = 2\delta_{\alpha,\alpha'} \frac{\gamma_\alpha T_\alpha}{\tau} \delta[\omega + \omega'], \quad \text{with} \quad \alpha, \alpha' = L, R \, . \tag{16}$$

Henceforth for convenience we will drop the subscript n from ω_n. Taking the Fourier transform of (4) gives the velocity vector in frequency domain as

$$\widetilde{V}(\omega) = i\omega \boldsymbol{G}^+ \, \widetilde{\eta} + \frac{1}{\tau} \boldsymbol{G}^+ (\, \boldsymbol{\Phi}\Delta X_\tau - i\omega \boldsymbol{M}\Delta V_\tau \,), \tag{17}$$

$$\text{where} \quad \Delta X_\tau = X(\tau) - X(0), \ \Delta V_\tau = V(\tau) - V(0) \, ,$$

and the Green's function matrix $\boldsymbol{G}^+(\omega)$ is given by (13). Since $\widetilde{\eta} \sim 1/\tau^{1/2}$ and ΔX_τ, ΔV_τ have finite variances for large τ, it follows that the second term in (17) is $O(1/\tau^{1/2})$ smaller than the first. As will be shown in the next section they contribute to the correction term $g(\lambda)$. In this section we focus on computing $\mu(\lambda)$ and the first term in (17) then gives:

$$\widetilde{v}_1(\omega) \sim i\omega[G_{1,1}^+(\omega) \, \widetilde{\eta}_L(\omega) + G_{1,N}^+(\omega) \, \widetilde{\eta}_R(\omega)] \, . \tag{18}$$

In terms of the Fourier transform, the expression in (6) for the heat transfer becomes

$$Q(\tau) = \tau \sum_{n=-\infty}^{\infty} \widetilde{q}_n \quad \text{with} \quad \widetilde{q}_n = \widetilde{\eta}_L(\omega)\widetilde{v}_1(-\omega) - \gamma_L \widetilde{v}_1(\omega)\widetilde{v}_1(-\omega). \tag{19}$$

For a chain with at least one pinned site it is easily seen from (18) that $\widetilde{v}_1(0) = 0$ and hence the heat transfer $\widetilde{q}_0$ through the zero-th mode vanishes in (19). This is related to the fact that for a pinned system there is no zero-frequency mode available

for transporting energy. Substituting (18) in (19) we write $Q(\tau) = \tau \sum_{n=1}^{\infty} (\tilde{q}_n + \tilde{q}_{-n})$ and using the fact $\tilde{\eta}_\alpha(-\omega) = \tilde{\eta}_\alpha^*(\omega)$ we get:

$$Z(\lambda) = \langle e^{-\lambda Q} \rangle \sim \prod_{n=1}^{\infty} \left\langle e^{-\lambda \tau \xi_n^T \boldsymbol{A}_n \xi_n^*} \right\rangle , \tag{20}$$

where $\xi_n = \left(\tilde{\eta}_L(\omega), \tilde{\eta}_R(\omega) \right)^T$

and $\boldsymbol{A}_n = \begin{pmatrix} 2\gamma_R \omega^2 |G_{1,N}^+|^2 & -i\omega G_{1,N}^- - 2\gamma_L \omega^2 G_{1,1}^+ G_{1,N}^- \\ i\omega G_{1,N}^+ - 2\gamma_L \omega^2 G_{1,1}^- G_{1,N}^+ & -2\gamma_L \omega^2 |G_{1,N}^+|^2 \end{pmatrix} , \tag{21}$

where in obtaining the $(1,1)^{\text{th}}$ element above we have made use of the identity

$$- \text{Im} G_{1,1}^+(\omega) = \omega \left[\gamma_L |G_{1,1}^+(\omega)|^2 + \gamma_R |G_{1,N}^+(\omega)|^2 \right] , \tag{22}$$

which can be proved as follows. From the definition of the Green's function in (13) we have $[\boldsymbol{G}^+]^{-1} - [\boldsymbol{G}^-]^{-1} = 2i\omega\boldsymbol{\gamma}$. Multiplying both sides by $\boldsymbol{G}^+$ from the left, and by $\boldsymbol{G}^-$ from the right we get $\boldsymbol{G}^- - \boldsymbol{G}^+ = 2i\omega\boldsymbol{G}^+ \boldsymbol{\gamma} \boldsymbol{G}^-$. The $(1,1)^{\text{th}}$ element of this leads to (22). For each n, the average in (20) is evaluated with respect to the Gaussian distribution

$$p(\xi_n) = \frac{1}{\pi^2 \det \boldsymbol{D}} \exp\left(-\xi_n^T \boldsymbol{D}^{-1} \xi_n^* \right) , \quad \text{with} \quad \boldsymbol{D} = \text{diag}\left(\frac{2d_L}{\tau}, \frac{2d_R}{\tau} \right) . \tag{23}$$

Hence we get (see Appendix B)

$$\left\langle e^{-\lambda\tau \xi_n^T \boldsymbol{A}_n \xi_n^*} \right\rangle = \left[\det(\boldsymbol{I} + \lambda\tau \boldsymbol{D}\boldsymbol{A}_n) \right]^{-1} , \tag{24}$$

$$= \left[1 + \mathcal{T}(\omega) T_L T_R \, \lambda(\Delta\beta - \lambda) \right]^{-1}, \tag{25}$$

where $\mathcal{T}(\omega)$ is given by (12). Using (20,25) and noting that in the $\tau \to \infty$ limit we can replace the summation over n by an integral over ω we obtain our final result in (11).

We remark that, the result (11) is in fact valid for both pinned as well as unpinned cases. For the unpinned harmonic system the centre of mass coordinate does not reach a steady state and it is useful to separate out this degree of freedom. Let us define new relative coordinates $y_l = x_l - x_N$, $l = 1, 2, \ldots, N-1$. The facts that the unpinned system has translational symmetry and that $\boldsymbol{\Phi}$ is a symmetric matrix imply the relation $\sum_{l=1,N} \Phi_{l,j} = \sum_{j=1,N} \Phi_{l,j} = 0$. Using this we get from (4):

$$\dot{y}_l = v_l - v_N, \quad l = 1, 2, \ldots, N-1 \tag{26}$$

$$m_l \dot{v}_l = -\sum_{j=1}^{N-1} \Phi_{l,j} y_j - \gamma_{l,l} v_l + \eta_l(t), \quad l = 1, 2, \ldots, N . \tag{27}$$

The relative coordinates y_l, $l = 1, 2, \ldots, N-1$ attain steady state with finite variance and it follows then from (26) that $\tilde{v}_l(\omega = 0) \sim \tilde{v}_N(\omega = 0)$ up to order $O(1/\tau)$. Then from (27) we get $\tilde{v}_l(0) \sim [\tilde{\eta}_L(0) + \tilde{\eta}_R(0)]/[\gamma_L + \gamma_R]$ for all l. We use this to compute the $\tilde{q}_0 \neq 0$ term in (19). With $\xi_0 = (\tilde{\eta}_L(0), \tilde{\eta}_R(0))^T$, we get

$$\tilde{q}_0 \sim \frac{1}{2} \xi_0^T \boldsymbol{A}_0 \xi_0 \quad \text{where} \quad \boldsymbol{A}_0 = \begin{pmatrix} \frac{2\gamma_R}{(\gamma_L+\gamma_R)^2} & -\frac{\gamma_L-\gamma_R}{(\gamma_L+\gamma_R)^2} \\ -\frac{\gamma_L-\gamma_R}{(\gamma_L+\gamma_R)^2} & -\frac{2\gamma_L}{(\gamma_L+\gamma_R)^2} \end{pmatrix} . \tag{28}$$

The noise ξ_0 has the Gaussian distribution

$$p(\xi_0) = \frac{1}{2\pi\sqrt{\det \boldsymbol{D}}} \exp\left(-\frac{1}{2}\xi_0^T \boldsymbol{D}^{-1}\xi_0\right) \tag{29}$$

and hence we get

$$\left\langle e^{-\lambda\tau\tilde{q}_0}\right\rangle \sim \left[\det(\boldsymbol{I} + \lambda\tau\boldsymbol{DA}_0)\right]^{-1/2} = \left[1 + \mathcal{T}(0)T_L T_R \lambda(\Delta\beta - \lambda)\right]^{-1/2} \tag{30}$$

where $\mathcal{T}(0) = 4\gamma_L\gamma_R/(\gamma_L + \gamma_R)^2$ is precisely what one obtains by taking $\mathcal{T}(\omega \to 0)$ in (12) for the unpinned system. This follows from the fact that in this case $G_{1N}^+|_{\omega\to 0} \sim 1/i\omega(\gamma_L + \gamma_R)$, a result which we now prove: For any matrix $\boldsymbol{A}$ let $\boldsymbol{A}_{(k,l)}^{(i,j)}$ denote the submatrix of $\boldsymbol{A}$ that occurs between the $(i,j)^{\text{th}}$ and the $(k,l)^{\text{th}}$ elements. Also let $\boldsymbol{B} = -\boldsymbol{M}\omega^2 + \boldsymbol{\Phi} + i\omega\boldsymbol{\gamma}$. Then we have $G_{1,N}^+ = (-1)^{N+1}\det\boldsymbol{B}_{(N-1,N)}^{(1,2)}\big/\det\boldsymbol{B}$. Taylor expanding the determinants about $\omega = 0$ we obtain $\det\boldsymbol{B}_{(N-1,N)}^{(1,2)} = \det\boldsymbol{\Phi}_{(N-1,N)}^{(1,2)} + O(\omega)$ and $\det\boldsymbol{B} = i\omega\gamma_L\det\boldsymbol{\Phi}_{(N,N)}^{(2,2)} + i\omega\gamma_R\det\boldsymbol{\Phi}_{(N-1,N-1)}^{(1,1)} + O(\omega^2)$, where we have used $\det\boldsymbol{\Phi} = 0$ that follows from the property $\sum_{l=1,N}\Phi_{l,j} = \sum_{j=1,N}\Phi_{l,j} = 0$. Using the latter property it is easy to show that $\det\boldsymbol{\Phi}_{(N,N)}^{(2,2)} = \det\boldsymbol{\Phi}_{(N-1,N-1)}^{(1,1)} = (-1)^{N-1}\det\boldsymbol{\Phi}_{(N-1,N)}^{(1,2)}$. Hence we get the desired result.

4. Calculation of $g(\lambda)$

We turn now to the more difficult problem of calculating $g(\lambda)$ which requires one to keep the second term in (17) and perform the average over initial conditions, in addition to the noise average. We recall that the heat transfer is given by (19) where the velocity $\tilde{v}_1$ can be obtained from the following exact solution for $\widetilde{X}, \widetilde{V}$:

$$\widetilde{X} = \boldsymbol{G}^+\tilde{\eta} - \frac{1}{\tau}\boldsymbol{G}^+\left(i\omega\boldsymbol{M}\Delta X_\tau + \boldsymbol{\gamma}\Delta X_\tau + \boldsymbol{M}\Delta V_\tau\right),$$

$$\widetilde{V} = i\omega\boldsymbol{G}^+\tilde{\eta} + \frac{1}{\tau}\boldsymbol{G}^+\left(\boldsymbol{\Phi}\Delta X_\tau - i\omega\boldsymbol{M}\Delta V_\tau\right), \tag{31}$$

$$\text{where } \Delta X_\tau = X(\tau) - X(0), \ \Delta V_\tau = V(\tau) - V(0).$$

To obtain $Z(\lambda) = \langle e^{-\lambda Q}\rangle$ we need to average over both noise $\tilde{\eta}$ and over the initial steady state distribution of U_0. We note that the solution in (31) contains $U^T(\tau) = (X^T(\tau), V^T(\tau))$ and this has to be expressed in terms of $\tilde{\eta}$ and U_0. While this can be done we follow a different strategy which is more convenient.

It is easier to calculate the restricted generating function

$$Z(\lambda, U, \tau|U_0) = \left\langle e^{-\lambda Q}\delta(U - U(\tau))\right\rangle_{U_0}, \tag{32}$$

where the average is performed only over noise and for a given initial condition U_0. We can then obtain $Z(\lambda) = \int dU \int dU_0 P_{\text{SS}}(U_0)Z(\lambda, U, \tau|U_0)$. The steps of the calculation now are as follows. We first note that, because of the δ-function constraint in (32), we can obtain Q as a quadratic function of the variables $\tilde{\eta}, U, U_0$. This follows from (19)

by using the following expression for $\tilde{v}_1(\omega)$ obtained from (31) by replacing $U(\tau)$ by U:

$$\tilde{v}_1(\omega) = i\omega[\ G_{11}^+\ \tilde{\eta}_L + G_{1N}^+\ \tilde{\eta}_R\ ] + \frac{1}{\tau}\sum_{l=1,N}[(\boldsymbol{G}^+\boldsymbol{\Phi})_{1l}\Delta X_l - i\omega(\boldsymbol{G}^+\boldsymbol{M})_{1l}\Delta V_l]$$

$$= i\omega[\ G_{11}^+\ \tilde{\eta}_L + G_{1N}^+\ \tilde{\eta}_R\ ] + \frac{1}{\tau}F_1^T\Delta U\ , \tag{33}$$

where

$$\Delta X = X - X(0),\ \ \Delta V = V - V(0),\ \ \Delta U = U - U(0),\ \ \ \text{and}$$

$$F_1^T\ =\ \left([\boldsymbol{G}^+\boldsymbol{\Phi}]_{1,1}, [\boldsymbol{G}^+\boldsymbol{\Phi}]_{1,2}, \ldots, [\boldsymbol{G}^+\boldsymbol{\Phi}]_{1,N}, -i\omega[\boldsymbol{G}^+\boldsymbol{M}]_{1,1}, -i\omega[\boldsymbol{G}^+\boldsymbol{M}]_{1,2}, \ldots, -i\omega[\boldsymbol{G}^+\boldsymbol{M}]_{1,N}\right)\ . \tag{34}$$

We replace the δ-function in (32) by the integral representations: $\delta(U - U(\tau)) = \int d^{2N}\sigma/(2\pi)^{2N}\ e^{i\sigma^T(U-U(\tau))}$ where $\sigma^T = (\sigma_1, \sigma_2, \ldots\sigma_{2N})$. We then have:

$$Z(\lambda, U, \tau|, U_0) = \int\frac{d^{2N}\sigma}{(2\pi)^{2N}}\ e^{i\sigma^T U}\langle e^{E(\tau)}\rangle_{U,U_0} \tag{35}$$

where $E(\tau) = -\lambda Q - i\sigma^T U(\tau)$.

We need an expression for $U^T(\tau) = (X^T(\tau),\ V^T(\tau))$ which we now obtain. We note that since we are using a Fourier-series representation for $X(t), V(t)$, the correct value at time τ is obtained from the Fourier-series by setting $t = \tau - \epsilon,\ \epsilon > 0$ and taking the limit $\epsilon \to 0$. Hence we obtain:

$$U^T = (\ X^T(\tau),\ V^T(\tau)\ ) = \lim_{\epsilon\to 0}\sum_{n=-\infty}^{\infty}\left(\ \widetilde{X}^T(\omega_n),\ \widetilde{V}^T(\omega_n)\ \right)\ e^{-i\omega_n\epsilon}\ .$$

For large τ we note that $(1/\tau)\sum_n\boldsymbol{G}^+(\omega_n)e^{-i\omega_n\epsilon} = 0$ which follows from converting the summation into a integral and noting that all the poles of $G^+(\omega_n)$ lie in the upper half plane. Hence we get:

$$U^T(\tau) = (\ X^T(\tau),\ V^T(\tau)\ ) = \sum_{n=-\infty}^{\infty}\left(\ [\boldsymbol{G}^+\tilde{\eta}]^T,\ i\omega[\boldsymbol{G}^+\tilde{\eta}]^T\ \right)\ e^{-i\omega_n\epsilon}$$

$$= \sum_{n=-\infty}^{\infty} e^{-i\omega_n\epsilon}\left[F_2^T\tilde{\eta}_L + F_3^T\tilde{\eta}_R\right]\ , \tag{36}$$

where

$$F_2^T = \left(G_{1,1}^+,\ G_{2,1}^+,\ \ldots, G_{N,1}^+,\ i\omega G_{1,1}^+,\ i\omega G_{2,1}^+, \ldots, i\omega G_{N,1}^+\right), \tag{37}$$

$$F_3^T = \left(G_{1,N}^+,\ G_{2,N}^+, \ldots, G_{N,N}^+,\ i\omega G_{1,N}^+,\ i\omega G_{2,N}^+, \ldots, i\omega G_{N,N}^+\right)\ . \tag{38}$$

Hence we get $E(\tau)$ in (35) as

$$E(\tau) = -\lambda Q - i\sum_{n=-\infty}^{\infty} e^{-i\omega_n\epsilon}\left[\sigma^T F_2\ \tilde{\eta}_L + \sigma^T F_3\ \tilde{\eta}_R\right]\ . \tag{39}$$

After using the full expression for $\widetilde{v}_1(\omega)$ from (33) to evaluate Q in (19), we obtain $E(\tau) = s_0 + \sum_{n=1}^{\infty}(s_n + s_{-n})$ where $(s_n + s_{-n})$ has the following quadratic form

$$s_n + s_{-n} = -\ \lambda\tau\xi_n^T\boldsymbol{A}_n\xi_n^* + \xi_n^T\alpha_n + \alpha_{-n}^T\xi_n^* + \frac{2\lambda\gamma_L}{\tau}|f_n|^2\ , \tag{40}$$

where the matrix $\boldsymbol{A}_n$ is given by (21) and

$$\alpha_n = \lambda \begin{pmatrix} 2i\gamma_L \omega G^+_{1,1} - 1 \\ 2i\gamma_L \omega G^+_{1,N} \end{pmatrix} F^\dagger_1 \Delta U - ie^{-i\omega\epsilon} \begin{pmatrix} F^T_2 \sigma \\ F^T_3 \sigma \end{pmatrix} , \tag{41}$$

$$f_n = F^T_1 \Delta U, \tag{42}$$

where F_1, F_2 and F_3 are given by (34),(37) and (38) respectively.

Similarly, one can express s_0 as

$$s_0 = -\frac{\lambda\tau}{2}\xi^T_0 \boldsymbol{A}_0 \xi_0 + \alpha^T_0 \xi_0 + \frac{\lambda\gamma_L}{\tau}f^2_0, \tag{43}$$

where $\boldsymbol{A}_0, \alpha_0, \xi_0$ and f_0 are all real.

We now first evaluate averages with respect to the Gaussian distribution given in (23) for $n \neq 0$ and with distribution given in (29) for $n = 0$. We get

$$\langle e^{(s_n + s_{-n})}\rangle_{U,U_0} = \frac{1}{\det(\boldsymbol{I} + \lambda\tau\boldsymbol{DA}_n)} \exp\left[\alpha^T_{-n}(\boldsymbol{D}^{-1} + \lambda\tau\boldsymbol{A}_n)^{-1}\alpha_n + \frac{2\lambda\gamma_L}{\tau}|f_n|^2 \right] \quad n \neq 0,$$

$$\langle e^{s_0}\rangle_{U,U_0} = \frac{1}{\sqrt{\det(\boldsymbol{I} + \lambda\tau\boldsymbol{DA}_0)}} \exp\left[\frac{1}{2}\alpha^T_0(\boldsymbol{D}^{-1} + \lambda\tau\boldsymbol{A}_0)^{-1}\alpha_0 + \frac{\lambda\gamma_L}{\tau}|f_0|^2 \right] . \tag{44}$$

Hence we get

$$\langle e^{E(\tau)}\rangle_{U,U_0} = \exp\left(-\frac{1}{2}\sum_{n=-\infty}^{\infty} \ln\left[\det(\boldsymbol{I} + \lambda\tau\boldsymbol{DA}_n) \right] \right)$$

$$\times \exp\left(\sum_{n=-\infty}^{\infty} \left[\frac{1}{2}\alpha^T_{-n}(\boldsymbol{D}^{-1} + \lambda\tau\boldsymbol{A}_n)^{-1}\alpha_n + \frac{\lambda\gamma_L}{\tau}|f_n|^2 \right] \right) \tag{45}$$

After evaluating the required matrix inverse and determinant, we take the large τ limit to replace all the summations over n by integrations over ω. This yields

$$\langle e^E\rangle_{U,U_0} \sim e^{\tau\mu(\lambda)} \exp\left(\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left[\frac{d_L d_R \, \alpha^T(-\omega)\boldsymbol{C}(\omega)\alpha(\omega)}{1 + T_L T_R \lambda(\Delta\beta - \lambda)\mathcal{T}(\omega)} + \lambda\gamma_L|f(\omega)|^2 \right] \right) ,$$

where $\mu(\lambda)$ is given by (11) and

$$\boldsymbol{C}(\omega) = \begin{pmatrix} \frac{1}{d_R} - 4\lambda\gamma_L\omega^2|G^+_{1,N}|^2 & 4\lambda\gamma_L\omega^2 G^+_{1,1}G^-_{1,N} + 2i\lambda\omega G^-_{1,N} \\ 4\lambda\gamma_L\omega^2 G^-_{1,1}G^+_{1,N} - 2i\lambda\omega G^+_{1,N} & \frac{1}{d_L} + 4\lambda\gamma_R\omega^2|G^+_{1,N}|^2 \end{pmatrix}. \tag{46}$$

We see from (41,42) that $\alpha(\omega)$, $f(\omega)$ are linear in ΔU and σ. After some algebraic manipulations and use of the identity (22) we then arrive at the following compact expression for $\langle e^E\rangle_{U,U_0}$:

$$\langle e^E\rangle_{U,U_0} \sim e^{\tau\mu(\lambda)} \exp\left(-\frac{1}{2}\sigma^T\boldsymbol{H}_1\,\sigma + i\Delta U^T\boldsymbol{H}_2\,\sigma + \frac{1}{2}\Delta U^T\boldsymbol{H}_3\,\Delta U \right), \tag{47}$$

where

$$\boldsymbol{H}_1(\lambda) = \frac{1}{2}(\,\boldsymbol{I}_1 + \boldsymbol{I}^T_1\,) , \tag{48}$$

with $\quad \boldsymbol{I}_1(\lambda) = \dfrac{d_L d_R}{\pi} \displaystyle\int_{-\infty}^{\infty} d\omega \, \dfrac{C_{1,1}F_2 F^\dagger_2 + C_{1,2}F_3 F^\dagger_2 + C_{2,1}F_2 F^\dagger_3 + C_{2,2}F_3 F^\dagger_3}{1 + T_L T_R \lambda(\Delta\beta - \lambda)\mathcal{T}(\omega)} ,$

$$\boldsymbol{H}_2(\lambda) = \lim_{\epsilon \to 0} \frac{\lambda}{\pi} \int_{-\infty}^{\infty} d\omega \, \mathrm{e}^{i\omega\epsilon} \frac{d_L(1 - 2i\omega\gamma_L \boldsymbol{G}_{1,1}^+)F_1^* F_2^\dagger - 2i\omega(\gamma_L + \lambda d_L)d_R \, \boldsymbol{G}_{1,N}^+ F_1^* F_3^\dagger}{1 + T_L T_R \lambda(\Delta\beta - \lambda)\mathcal{T}(\omega)} \,, \quad (49)$$

and

$$\boldsymbol{H}_3(\lambda) = \frac{1}{2}\left(\, \boldsymbol{I}_3 + \boldsymbol{I}_3^T \,\right) , \quad (50)$$

with $\qquad \boldsymbol{I}_3(\lambda) = \frac{\lambda(\gamma_L + \lambda d_L)}{\pi} \int_{-\infty}^{\infty} d\omega \, \frac{F_1 F_1^\dagger}{1 + T_L T_R \lambda(\Delta\beta - \lambda)\mathcal{T}(\omega)} \,.$

Finally to get $Z(\lambda, U, \tau|U_0)$ we substitute the expression for $\langle \mathrm{e}^E \rangle_{U,U_0}$ from (47) into (35) and perform the Gaussian integration over σ. This gives

$$Z(\lambda, U, \tau|U_0) \sim \frac{\mathrm{e}^{\tau\mu(\lambda)}}{(2\pi)^N \sqrt{\det \boldsymbol{H}_1}} \, \mathrm{e}^{\frac{1}{2}\Delta U^T \boldsymbol{H}_3 \, \Delta U} \, \mathrm{e}^{-\frac{1}{2}(U^T + \Delta U^T \boldsymbol{H}_2)\boldsymbol{H}_1^{-1}(U + \boldsymbol{H}_2^T \Delta U)}. \quad (51)$$

Putting $\lambda = 0$ in the above expression gives the steady state distribution as

$$P_{\mathrm{SS}}(U) = Z(0, U, \tau \to \infty|U_0) = \frac{\exp\left(-\frac{1}{2}U^T \boldsymbol{H}_1^{-1}(0)U\right)}{(2\pi)^N \sqrt{\det \boldsymbol{H}_1(0)}} \,. \quad (52)$$

From the long time solution in (36) it can be directly verified that

$$\lim_{t \to \infty} \langle UU^T \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \left[d_L F_2 F_2^\dagger + d_R F_3 F_3^\dagger \right] ,$$

and using the fact that $\langle UU^T \rangle$ is real we see that the above equals $\boldsymbol{H}_1(0)$, consistent with (52)

Now, according (8), the initial and the final variables U_0 and U in (51) must factorize, which implies $[\boldsymbol{H}_3 - \boldsymbol{H}_2 \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T - \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T] + [\boldsymbol{H}_3 - \boldsymbol{H}_2 \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T - \boldsymbol{H}_2 \boldsymbol{H}_1^{-1}]^T = \boldsymbol{0}$. Since $\boldsymbol{H}_1$ and $\boldsymbol{H}_3$ are symmetric matrices, the above condition can be expressed as

$$\boldsymbol{H}_3 - \boldsymbol{H}_2 \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T - \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T = \boldsymbol{0} \,, \quad (53)$$

Using this (51) gives

$$Z(\lambda, U, \tau|, U_0) \sim \frac{\mathrm{e}^{\tau\mu(\lambda)}}{(2\pi)^N \sqrt{\det \boldsymbol{H}_1(\lambda)}} \exp\left(-\frac{1}{2}U^T \boldsymbol{L}_1(\lambda)U\right) \exp\left(-\frac{1}{2}U_0^T \boldsymbol{L}_2(\lambda)U_0\right) . \quad (54)$$

This means that we can make the following identifications for $\Psi(U, \lambda)$, $\chi(U_0, \lambda)$:

$$\Psi(U, \lambda) = \frac{1}{(2\pi)^N \sqrt{\det \boldsymbol{H}_1(\lambda)}} \, \exp\left(-\frac{1}{2}U^T \boldsymbol{L}_1(\lambda)U\right) , \quad (55)$$

$$\chi(U_0, \lambda) = \exp\left(-\frac{1}{2}U_0^T \boldsymbol{L}_2(\lambda)U_0\right) , \quad (56)$$

where $\qquad \boldsymbol{L}_1(\lambda) = \boldsymbol{H}_1^{-1} + \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T \qquad\qquad\qquad\qquad\qquad (57)$

and $\qquad \boldsymbol{L}_2(\lambda) = \boldsymbol{H}_2 \boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T - \boldsymbol{H}_3 = -\boldsymbol{H}_1^{-1} \boldsymbol{H}_2^T \,. \qquad\qquad\qquad (58)$

Thus we have obtained the left and right eigenvectors of the Fokker-Planck operator $\mathcal{L}_\lambda$ corresponding to the eigenvalue $\mu(\lambda)$. It can be seen that the orthonormality condition $\int dU \chi(U, \lambda)\Psi(U, \lambda) = 1$ is satisfied.

We obtain $Z(\lambda)$ by integrating $Z(\lambda, U, \tau|U_0)$ over U and then averaging over the initial condition U_0 with respect to the steady state distribution $P_{SS}(U_0)$. This then gives our final expression for the correction to the CGF:

$$g(\lambda) = \left(\det \boldsymbol{H}_1(\lambda) \det \boldsymbol{H}_1(0) \det \boldsymbol{L}_1(\lambda) \det[\boldsymbol{H}_1^{-1}(0) + \boldsymbol{L}_2(\lambda)] \right)^{-1/2}. \quad (59)$$

Since $\boldsymbol{L}_1(0) = \boldsymbol{H}_1^{-1}(0)$ and $\boldsymbol{L}_2(0) = \boldsymbol{0}$, it is verified that $g(0) = 1$.

5. Example of Single Brownian particle

The Langevin equation for a single Brownian particle is given by :

$$m\dot{v} = -(\gamma_L + \gamma_R)v + \eta_L(t) + \eta_R(t), \quad (60)$$

where v is the velocity of the particle and m is it's mass. Here we consider the velocity of the particle not the position since velocity v of the particle will have a normalized steady state distribution whereas position will not have and the heat transfer Q, in which we are interested, does not depend on position. For single Brownian particle the matrix defined in (13) becomes a complex number: $\boldsymbol{G}^+(\omega) = 1/(-m\omega^2 + i\omega\gamma)$ where $\gamma = \gamma_L + \gamma_R$. Following all the steps described in the last section one can easily arrive at the expression (47) where, $\mu(\lambda)$ is given in (11) and $\boldsymbol{H}$'s are given in (48), (49) and (50). In this case one can carry out the integrations present in the expressions of all these quantities. The expression for phonon transmission coefficient is obtained from (12) and given by $\mathcal{T}(\omega) = 4\gamma_L\gamma_R[m^2\omega^2 + (\gamma_L + \gamma_R)^2]^{-1}$. We use this form in (11) to evaluate the integral and get

$$\mu(\lambda) = \frac{\gamma_L + \gamma_R}{2m} \left[1 - \sqrt{1 + \frac{4\gamma_L\gamma_R}{(\gamma_L + \gamma_R)^2} T_L T_R \lambda(\Delta\beta - \lambda)} \right]. \quad (61)$$

This is the result obtained in [16]. Similarly using $\boldsymbol{G}^+(\omega) = 1/(-m\omega^2 + i\omega\gamma)$ and the above form for $\mathcal{T}(\omega)$ we evaluate $\boldsymbol{H}$'s given by (48), (49) and (50) to get

$$\boldsymbol{H}_1 = \frac{d_L + d_R}{m\sqrt{\gamma^2 + a^2}},$$

$$\boldsymbol{H}_2 = \frac{\lambda d_L + \frac{1}{2}(\gamma - \sqrt{\gamma^2 + a^2})}{\sqrt{\gamma^2 + a^2}},$$

$$\boldsymbol{H}_3 = \frac{m\lambda}{\sqrt{\gamma^2 + a^2}} \left(\gamma_L + \lambda d_L \right),$$

where, $\quad a = \sqrt{4d_L d_R \lambda(\Delta\beta - \lambda)}. \quad (62)$

It is easily verified that $\boldsymbol{H}$s' for the single Brownian particle satisfy the relation (53), i.e. $(\boldsymbol{H}_2)^2 + \boldsymbol{H}_2 - \boldsymbol{H}_1\boldsymbol{H}_3 = 0$. Now using the expression (59) we obtain

$$g(\lambda) = 2\sqrt{\frac{\gamma\sqrt{\gamma^2 + 4d_L d_R \lambda(\Delta\beta - \lambda)}}{(\gamma + \sqrt{\gamma^2 + 4d_L d_R \lambda(\Delta\beta - \lambda)})^2 - 4\lambda^2 d_L^2}}, \quad (63)$$

which also agrees with the result in [16].

6. Discussions

We have presented a formalism to calculate the CGF $\mu(\lambda)$ and it's correction $g(\lambda)$ for heat transport across a harmonic chain connected to white-noise Langevin reservoirs. The formula for $\mu(\lambda)$ is expressed as an integral over frequencies, with the integrand depending explicitly on the phonon transmission function $\mathcal{T}(\omega)$. The expression for $g(\lambda)$ is in terms of integrals involving an appropriate phonon Green's function. We have illustrated the usefulness of the formalism by calculating $\mu(\lambda)$ and $g(\lambda)$ for a single Brownian particle for which case all integrals can be performed explicitly. For systems with more number of particles, the function $\mathcal{T}(\omega)$ can easily be obtained analytically for an ordered harmonic chain and numerically for disordered harmonic chains. Hence our formalism can be used to numerically compute $\mu(\lambda)$ and $g(\lambda)$ with high accuracy. A knowledge of these functions would enable one to check the validity of the fluctuation symmetry for the large deviation function. We note that $\mu(\lambda)$ itself is a useful quantity, containing information on current moments in the nonequilibrium state. We show that it always satisfies the fluctuation symmetry relation. Finally we have pointed out that $\mu(\lambda)$ can, in general, be shown to be the largest eigenvalue of a Fokker-Planck type operator ($\mathcal{L}_\lambda$ for our problem). Using our formalism we not only obtain this eigenvalue but also the corresponding left and right eigenvectors.

The present approach has recently been generalized to the problem of computing $\mu(\lambda)$ for the case of heat conduction across arbitrary harmonic networks [40]. The problem of calculating $g(\lambda)$ in such cases and also the extension of the present formalism to quantum systems are interesting open problems.

Appendix A. The Fokker-Planck equation

Let $P(Q, U, t|U_0)$ denotes the probability distribution of heat flow Q in duration τ given the initial and final configuration U and U_0 respectively. The distribution $P(Q, U, t|U_0)$ satisfies the following Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \Bigg[-\sum_{l=1}^{2N} \frac{\partial}{\partial U_l} \frac{\langle \Delta U_l \rangle}{\Delta t} - \frac{\partial}{\partial Q} \frac{\langle \Delta Q \rangle}{\Delta t} + \frac{1}{2} \sum_{l=1}^{2N} \sum_{m=1}^{2N} \frac{\partial^2}{\partial U_l \partial U_m} \frac{\langle \Delta U_l \Delta U_m \rangle}{\Delta t}$$

$$+ \sum_{l=1}^{2N} \frac{\partial^2}{\partial U_l \partial Q} \frac{\langle \Delta U_l \Delta Q \rangle}{\Delta t} + \frac{1}{2} \frac{\partial^2}{\partial Q^2} \frac{\langle \Delta Q^2 \rangle}{\Delta t} \Bigg] P(Q, U, t|U_0) \; ; \quad \text{with } \Delta t \to 0 \;, \qquad (A.1)$$

where the moments are calculated using the Langevin equations (4) and heat equation given in (6). After calculating the moments we get

$$\frac{\partial P}{\partial t} = \mathcal{L}_Q \; P(Q, U, t|U_0) \qquad (A.2)$$

where

$$\mathcal{L}_Q = \sum_{l=1}^{N} \frac{1}{m_l} \Big[\frac{\partial \mathcal{H}}{\partial x_l} \frac{\partial}{\partial v_l} - \frac{\partial \mathcal{H}}{\partial v_l} \frac{\partial}{\partial x_l} \Big]$$

$$+ \frac{\gamma_L}{m_1} \frac{\partial}{\partial v_1} v_1 + \frac{\gamma_R}{m_N} \frac{\partial}{\partial v_N} v_N + \left(\gamma_L v_1^2 - \frac{\gamma_L T_L}{m_1} \right) \frac{\partial}{\partial Q}$$

$$+ \frac{\gamma_L T_L}{m_1^2} \frac{\partial^2}{\partial v_1^2} + \frac{\gamma_R T_R}{m_N^2} \frac{\partial^2}{\partial v_N^2} + \gamma_L T_L v_1^2 \frac{\partial^2}{\partial Q^2} + \frac{2\gamma_L T_L}{m_1} \frac{\partial^2}{\partial v_1 \partial Q} v_1. \quad \text{(A.3)}$$

The corresponding Fokker-Planck equation for the restricted characteristic function $Z(\lambda, U, t|U_0) = \int_{-\infty}^{\infty} dQ \mathrm{e}^{-\lambda Q} P(Q, U, t|U_0)$ is obtained by multiplying both sides of the above equation by $\mathrm{e}^{-\lambda Q}$ and then integrating with respect to Q. We get

$$\frac{\partial}{\partial \tau} Z(\lambda, U, \tau|U_0) = \mathcal{L}_\lambda \ Z(\lambda, U, \tau|U_0) \quad \text{(A.4)}$$

where

$$\mathcal{L}_\lambda = \sum_{l=1}^{N} \frac{1}{m_l} \left[\frac{\partial \mathcal{H}}{\partial x_l} \frac{\partial}{\partial v_l} - \frac{\partial \mathcal{H}}{\partial v_l} \frac{\partial}{\partial x_l} \right]$$

$$+ \frac{\gamma_L}{m_1} \frac{\partial}{\partial v_1} v_1 + \frac{\gamma_R}{m_N} \frac{\partial}{\partial v_N} v_N + \left(\gamma_L v_1^2 - \frac{d_L}{m_1} \right) \lambda$$

$$+ \frac{d_L}{m_1^2} \frac{\partial^2}{\partial v_1^2} + \frac{d_R}{m_N^2} \frac{\partial^2}{\partial v_N^2} + d_L v_1^2 \lambda^2 + \frac{2d_L}{m_1} \lambda \frac{\partial}{\partial v_1} v_1. \quad \text{(A.5)}$$

Appendix B. Multidimensional Gaussian integral of complex variables

For ease of reference we give the following result for complex Gaussian integrals.

$$\int d^n Z \exp(-Z^T \boldsymbol{A} Z^* + Z^T B + C^T Z^*) = \frac{\pi^n}{\det \boldsymbol{A}} \exp(C^T \boldsymbol{A}^{-1} B) \quad \text{(B.1)}$$

where Z is a n-dimensional complex vector, $\boldsymbol{A}$ is a Hermitian matrix and B, C are arbitrary complex n-dimensional vectors. The integration $\int d^n Z$ denotes the real integrations $\int d^n X d^n Y$ with the substitution $Z = X + iY$, X and Y being real n-dimensional vectors.

Proof: Let $\boldsymbol{K}$ be the unitary matrix such that $\boldsymbol{A} = \boldsymbol{K} \boldsymbol{D} \boldsymbol{K}^\dagger$ where $\boldsymbol{D}$ is a diagonal matrix with all real diagonal elements. Now with the following transformations

$$\widetilde{Z} = \boldsymbol{K}^T Z \ , \widetilde{B} = \boldsymbol{K}^\dagger B \ , \ \widetilde{C} = \boldsymbol{K}^T C \quad \text{(B.2)}$$

we can write the complex Gaussian integration in the form

$$\int_{\infty}^{\infty} d^n \widetilde{X} d^n \widetilde{Y} \exp(-\widetilde{Z}^T \boldsymbol{D} \widetilde{Z}^* + \widetilde{Z}^T \widetilde{B} + \widetilde{C}^T \widetilde{Z}^*). \quad \text{(B.3)}$$

Since $\boldsymbol{D}$ is diagonal, the above is a product of $2n$ uncoupled Gaussian integrations. Performing the integrations we get:

$$\prod_{i=1}^{n} \frac{\pi}{D_i} \exp(\frac{\widetilde{B}_i \widetilde{C}_i}{D_i}) = \frac{\pi^n}{\det \boldsymbol{A}} \exp(\widetilde{C}^T \boldsymbol{D}^{-1} \widetilde{B}) = \frac{\pi^n}{\det \boldsymbol{A}} \exp(C^T \boldsymbol{A}^{-1} B) \ , \quad \text{(B.4)}$$

which completes the proof.

References

[1] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Phys. Rev. Lett. **71**, 2401 (1993).

[2] D. J. Evans and D. J. Searles, Phys. Rev. E **50**, 1645 (1994).

[3] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995).

[4] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).

[5] J. Kurchan, J. Phys. A: Math. Gen. **31**, 3719 (1998).

[6] G. E. Crooks, Phys. Rev. E **60**, 2721 (1999).

[7] J. L. Lebowitz and H. Spohn, J. Stat. Phys. **95**, 333 (1999).

[8] T. Hatano and S. Sasa, Phys. Rev. Lett. **86**, 3463 (2001).

[9] O. Narayan and A. Dhar, J. Phys. A: Math. Gen. **37** 63 (2004).

[10] U. Seifert, Phys. rev. lett. **95**, 040602, (2005).

[11] C. Jarzynski and D. K. Wojcik, Phys. Rev. Lett. **92**, 230602 (2004).

[12] T. Bodineau and B. Derrida, Phys. Rev. Lett. **92**, 180601 (2004).

[13] C. Enaud and B. Derrida, J. Stat. Phys. **114**, 537 (2004).

[14] B. Derrida, B. Doucot and P.-E. Roche J. Stat. Phys. **115**, 717-748 (2004).

[15] B. Derrida and J.L. Lebowitz, Phys. Rev. Lett. **80**, 209 (1998).

[16] P. Visco, J. Stat. Mech. P06006 (2006).

[17] K. Saito and A. Dhar, Phys. Rev. Lett. **99**, 180601 (2007).

[18] D. Andrieux and P. Gaspard, Phys. Rev. E 74, 011906 (2006).

[19] D. Lacoste, A. W.C. Lau, and K. Mallick, Phys. Rev. E **78**, 011915 (2008).

[20] G. M. Wang *et al* , Phys. Rev. Lett. **89**, 050601 (2002).

[21] D. M. Carberry *et al* , Phys. Rev. Lett. **92**, 140601 (2004).

[22] K. Feitosa and N. Menon, *i*bid **92**, 164301 (2004).

[23] W. I. Goldburg *et al* , Phys. Rev. Lett. **87**, 245502 (2001).

[24] F. Douarche *et al* , *i*bid **97**, 140603 (2006).

[25] J. Liphardt *et al* , Science **296**, 1832 (2002).

[26] D. Collin *et al* , Nature **437**, 231 (2005).

[27] J. R. Gomez-Solano *et al* , Europhys Lett. **89** 60003 (2010).

[28] S. Majumdar and A. K. Sood, Phys. Rev. Lett. **101**, 078301 (2008).

[29] H. Touchette, Phys. Rep. **478**, 1 (2009).

[30] A. Gomez-Marin and J. M. Sancho , Phys. Rev. E **73**, 045101(R),(2006).

[31] F. van Wijland, Phys. Rev. E **74**, 063101 (2006).

[32] J. Farago, J. Stat. Phys., **107**, 781 (2002).

[33] R. van Zon and E. G. D. Cohen, Phys. Rev. Lett. **91**, 110601 (2003); Phys. Rev. E **69**, 056121 (2004).

[34] Z. Rieder, J. L. Lebowitz and E. Lieb, J. Math. Phys. **8**, 1073 (1967).

[35] A. Dhar and D. Roy, J. Stat Phys. **125**, 801 (2006).

[36] A. Casher and J.L. Lebowitz, J. Math. Phys. **12**, 1701 (1971).

[37] A. Dhar, Phys. Rev. Lett. **86**, 5882 (2001).

[38] R. J. Rubin and W. L. Greer, J. Math. Phys. **12**, 1686 (1971).

[39] A. J. O'Connor and J. L. Lebowitz, J. Math. Phys. **15**, 692 (1974).

[40] K. Saito and A. Dhar, arXiv:1012.0622.